

7,7'-(Carbonyldiimino)bis[4-hydroxy-2-naphthalenesulfonic acid]
134-47-4 | DTXSID7059642

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.15

Global applicability domain: Outside

Local applicability domain index: 2.12e-01

Confidence level: 3.02e-01

Nearest Neighbors from the Training Set

Image not found

4,4'-Diamino-2,2'-stilbenedisulfonic acid

Measured: -1.70

Predicted: 3.09e-01

Image not found

Sulcofuron-sodium

Measured: 1.89

Predicted: 3.12